Guanidine, N,N'''-(iminodi-8,1-octanediyl)bis-

13516-27-3 | DTXSID7042015

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.53e-10 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.46e-01

Confidence level: 2.94e-01

Nearest Neighbors from the Training Set

Image not found
9,10-Anthracenedione, 1,4-bis(methylamino)-
Measured: 1.80e-08
Predicted: 4.57e-11

Image not found
1-Dodecanethiol
Measured: 8.00e-07
Predicted: 7.73e-03

Image not found
Lepidine
Measured: 8.02e-14
Predicted: 9.90e-03

Image not found
2,4,6-Trimethylpyridine
Measured: 3.59e-10
Predicted: 8.58e-01

Image not found
4-Chloro-3-methylphenol
Measured: 1.50e-12
Predicted: 5.35e-02